Three-dimensional boiling-water reactor neutron flux calculations on the basis of homogenized fuel box cross sections

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Three-dimensional Boiling-water Reactor Neutron Flux Calculations on the Basis of Homogenized Fuel Box Cross Sections

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Abstract

Three-dimensional overall calculations are set up with the SYNTRON/VOID program as whole core calculations on the Dresden 1 reactor. The utility of the methods used for the production of box average cross sections on the basis of separate fuel box calculations with the CDB code are investigated. An alternative method for the determination of box average diffusion constants is proposed.

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CONTENTS

Introduction

This report describes a series of investigations performed in order to clear up some of the difficulties observed in connection with the 3D overall calculations on the Dresden 1 reactor [1]. The investigations concern both the neutron - hydraulics calculation methods and the supply of cross sections, i.e. the methods used to produce equivalent box and control rod cross sections. When the calculations of ref. 1 were performed, the SYNTRON code [2] could treat only a quarter of the core. These limitations have now been removed, and it has become possible to set up a 3D overall calculation on the whole Dresden 1 reactor core in 2 energy groups and a number of mesh points of 48 x 48 in the radial directions and 36 in the axial direction. In these new calculations the reflector was replaced by a set of boundary conditions including up- and down-scattering, so-called gamma matrices, in order to save mesh points. The SYNTRON code was modified so that it was possible to use as many as 60 hydraulic channels, which in fact for the present case is one channel for every four fuel boxes, taking into account a half core rotational symmetry in the control rod positions.

The routine used for the calculations of the two-dimensional trial functions in SYNTRON by means of conventional finite difference techniques was greatly modified so that it is now possible to use more mesh points, namely a practical maximum of about 90 x 90 for a 2 energy group case.

The methods used for the production of box average cross sections on the basis of fuel box calculations with CDB[3] are discussed. The determination of average diffusion constants is investigated in order to get proper couplings between rodded and unrodded fuel boxes in the overall treatment in SYNTRON. Difficulties encountered in connection with the smearing out of the control rods over the whole fuel box are reported on.

The two different methods of represention of control rods and water gaps in the box calculation, i.e. as cross sections or boundary conditions, γ-matrices, are investigated. For a Dresden 1 fuel box the results of the two methods are in good agreement, within a few per cent in the power distribution and a few per mille in the k_{eff}.

As with the calculations of ref. 1 the data supply program is CRS[4]. However, since the calculations of ref. 1 several modifications of the CRS code have been implemented: One-dimensional collision probability spectrum calculations for the condensation of the cross sections, improved thermal scattering matrix treatment, and a correction to the removal cross sections of H in the resonance region; these modifications are described in ref. 5.

The calculations of this report were set up in order to investigate simultaneously the importance of all these improvements and modifications in the different codes necessary before setting up a full 3D overall calculation with SYNTRON.

2. γ-Matrices Used as Boundary Conditions in Finite Difference Schemes Taking the Flux Point in the Middle of the Mesh

In reactor physics diffusion theory calculations it is often convenient to replace some structural regions, for example control rods and reflectors, by a set of boundary conditions. This may be done either in the hope of getting better results or to save mesh points in the diffusion theory calculation.

One kind of boundary conditions often used at Risø are the so-called γ-matrices. The γ-matrix is simply defined as a full matrix

$$\bar{J} = \bar{\bar{\gamma}} \cdot \bar{\phi} \qquad (2.1)$$

Linking the current and the flux at the boundary, i.e. inclusive of up-and down-scattering. These γ-matrices may be calculated by the collision probability program HECS[6]. The method has earlier been mentioned in refs. 1 and 7. However, the use of γ-matrices as boundary conditions in finite difference schemes taking the flux point in the middle of the mesh, as for example CDB and SYNTRON, is somewhat problematic as the γ-matrix is related to the physical boundary, and the flux to the centre of the adjacent mesh. For that reason it is necessary to introduce the γ-matrix formalism with care in the finite difference scheme.

The following method was used for the γ-matrix representation in the SYNTRON program. The diagonal elements are treated as leakage terms, whereas the off-diagonal elements are transformed into equivalent up-and down-scattering cross sections in the adjacent meshes.

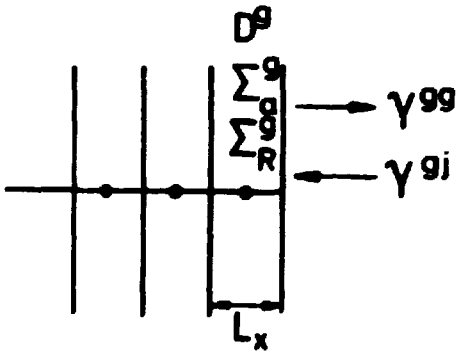


Fig. 2a. Gamma matrix representation

The leakage term DD^g, giving the total current out when multiplied by the neutron flux ϕ^g, is calculated in the following way:

$$DD^g = \frac{1}{\frac{1}{\gamma^{gg}} + \frac{Lx}{2D^g}} \; Ly . \qquad (2.2)$$

The scattering terms, i.e. the off-diagonal γ-matrix elements, are added to the scattering cross sections in the adjacent mesh. The scattering out of the group γ_R^g is added to the absorption term to give the total removal term, AT^g, in the mesh:

$$AT^g = \Sigma_a^g \; Lx \; Ly + \gamma_R^g \; Ly . \qquad (2.3)$$

The scattering elements are added to the scattering cross sections of the adjacent mesh to give the total scattering term, SS^{gj}, of the mesh.

$$SS^{gj} = \Sigma^{gj} \cdot Lx \cdot Ly - \gamma^{gj} \cdot Ly. \qquad (2.4)$$

The scattering-in and scattering-out term (2.3), (2.4) are set up as if the mesh adjacent to the boundary was infinitely narrow, assuming the same flux at the centre of the mesh as at the surface. In the leakage term (2.2) the diagonal γ-matrix element is treated as an extrapolation boundary, and the finite mesh sizes are taken into account. In fact the leakage term only represents the net loss from the group and not the scattering to other groups. In order to establish the correct neutron balance for the eigenvalue calculation it is important that what is leaving group g is equal to what is entering the other groups from group g.

In the γ-matrices calculated by the HECS [6] code the diagonal elements represent both the net loss and the removal, i.e. $\gamma^{gg} + \gamma_R^g$. For that reason it is natural to represent the total leakage in accordance with (2.2) with γ^{gg} replaced by $\gamma^{gg} + \gamma_R^g$. This representation was used in the CDB box code for calculations of ref. 1. However, the method gave erroneous results for cases with dominating scattering, for example a γ-matrix representing the water round a fuel box. In the case of infinitely narrow meshes the two methods merge as $DD^g \simeq \gamma^{gg} \cdot Ly$ in this case. For a finite mesh size the $\frac{Lx}{2D^g}$ correction to the γ_R^g term, but not to the γ^{gj} terms, will make the net loss undetermined and thus the eigenvalue erroneous.

The box calculations on a Dresden 1 fuel box with and without control rod as described in chapter 6 of ref. 1 was repeated with the corrected γ-matrix treatment in the CDB code. Furthermore an input error observed

in the case of a control rod represented by cross sections was corrected. The error may be observed by comparing fig. 6.1.a and fig. 3.3.b in ref. 1. The control rod has simply been smeared out over the adjacent water gap, and thus over-estimated. The error does not affect the calculation with a control rod represented by a γ -matrix.

The calculations were set up in order to compare the k_{eff} and the power distributions for a Dresden 1 fuel box with 25% void with the control rod and water gaps represented as macroscopic cross sections or γ-matrices. The fundamental cross sections for the box code were generated by the CRS code as in ref. 1, but since then some modifications have been introduced in the CRS code, and for that reason the cross sections used in ref. 1 and that used in these calculations differ slightly. It should be mentioned that the condensation of the transport cross section from 76-group structure in CRS to the 5-group structure of the overall box calculation is different in the two cases. The transport cross sections are inversely group-condensed when they are to be used as diffusion constants, whereas when they are to be used in the collision probability code HECS, for the γ -matrix production, they are directly group-condensed.

In table 2.a the calculated k_{eff}'s are presented. It may be seen that the k_{eff}'s are quite identical considering the accuracy of the calculation. As expected, the large deviation between the two methods reported in ref. 1 for the scattering dominated, unrodded fuel box, has disappeared.

Table 2.a

Calculated k_{eff}'s for a Dresden 1 fuel box with 25% void

	Control rod and water gaps Cross sec. repr.	Control rod and water gaps γ -matrix repr.
Rodded box	0.82397	0.82366
Unrodded box	1.1191	1.1206

Furthermore the unrodded case was calculated with the CDB diffusion routine replaced by the TVEDIM code [8], which is a diffusion code taking the flux points at the surface of the meshes, and therefore well suited for γ-matrix representation. The TVEDIM results were within 0.1 % of those of table 2.a.

The calculated power distributions are shown in fig. 2.b. For the un-

rodded case the deviation between the two results is within 1%. For the rodded fuel box the deviation is as much as 9% for the fuel pin in the corner adjacent to the control rod, whereas the deviations are less than 6% for the rest of the pin cells. It will be noted that the deviation between cross section and γ-matrix representation for the rodded fuel box is much less in these corrected calculations than in the erroneous calculations of ref. 1. However, as the error in the γ-matrix representation does not seriously affect the power distributions obtained, the comparison in ref. 1 of S_4 and γ-matrix-represented diffusion theory is still valid. The conclusions are that the errors introduced by using diffusion theory with cross-section-represented water gaps and control rods for the fuel box are only a few per cent larger than for diffusion theory with γ-matrix-represented water gaps and control rod compared with S_4 calculations. This conclusion is naturally only true when the macroscopic cross sections are produced on the basis of one-dimensional collision probability calculations, in 76 energy groups, to give the correct homogenization of the different regions for the effective cross section used in the box code, as performed in the CRS code.

One reason why one may prefer to represent the control rods and water gaps by cross sections is that the problem of homogenization of the box with γ-matrices involved to give average cross sections for later use in for instance 3D overall calculations, has still not been solved satisfactorily.

The use of γ-matrices as boundary conditions seems very attractive in 3D overall calculations to replace the reflector, core baffle, and so on. The purpose may be to save mesh points, or get better results with the same total number of mesh points. In ref. 9 an infinitely thick light-water reflector was replaced by the corresponding γ-matrix, with an enormous saving of mesh points and consequently of computer time, and the calculated k_{eff}'s differ less than 0.2%.

For reactors where the reflector consists of consecutive layers of steel and water it is very desirable to replace such a complicated structure by one set of boundary conditions in the 3D calculations.

Several test calculations in two dimensions with SYNTRON were set up in connection with the calculations on the Dresden 1 reactor in order to compare the results obtained by direct cross section representation of the reflector with γ-matrix representation. All these calculations gave deviations in the calculated eigenvalues of only about 0.1-0.2%, and only a few per cent's deviation in the flux distributions in the boxes adjacent to the reflector. However, the most important observation is that the results calculated with γ-matrices on the reflector are more accurate in comparison with detailed

Top : cros section repr.

Bottom: γ - matrix repr.

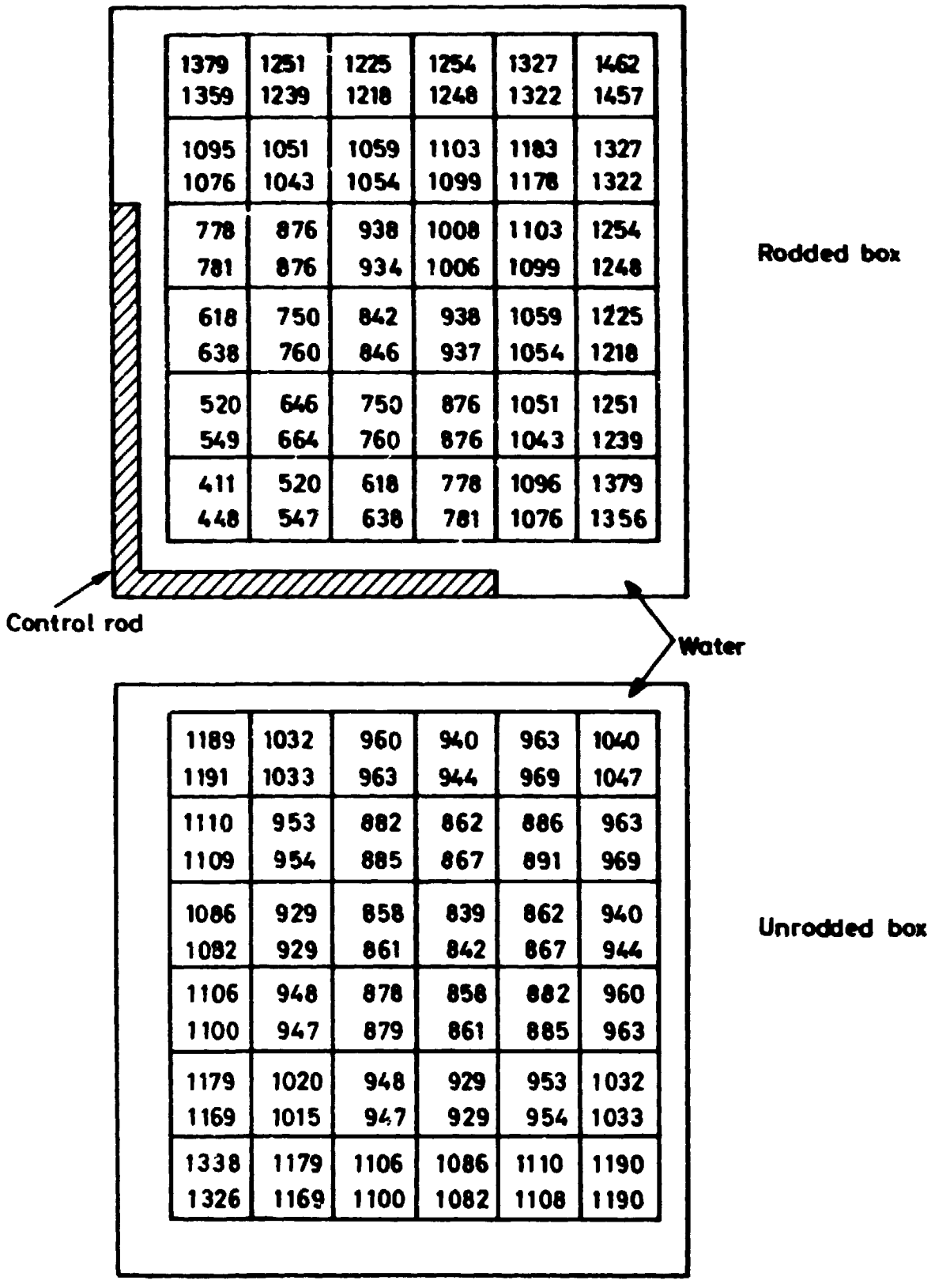


Fig. 2b. Dresden 1 fuel box, 25% void, with and without control rod. Comparison between cross section and γ-matrix representation.

2D calculations with 90 x 90 mesh points than the calculations with cross sections on the reflector and with the same total number of mesh points.

3. Production of Box-averaged Effective Cross Sections and Diffusion Constants

In this chapter the methods used for the production of effective box--averaged macroscopic cross sections and diffusion constants to be used in 3-dimensional diffusion theory calculations will be investigated and discussed.

The homogenization of parts of the reactor core, for example the fuel boxes surrounded by water gaps and control rods, facilitates the overall calculation. In fact overall calculations with direct representation of control rods and water gaps demand lots of regions of alternating properties and dimensions: water, control rods, fuel unit cells, and so on. If reasonable results are to be obtained on such a system finite difference calculations are only possible if small mesh sizes are used, about one mesh point per unit cell. Two-dimensional calculations of that type are large but possible, whereas three-dimensional calculations seem beyond computation.

A suitable unit for homogenization is the fuel box surrounded by control rod and separating water. This homogenization may be performed on the basis of transport calculations or other refined methods, and when the different regions are represented by average cross sections, the properties throughout the reactor in the finite difference calculation are much smoother and consequently allow the use of a coarser mesh division.

When the methods of homogenized cross sections are used, it is naturally only possible to calculate average quantities for the fuel boxes. However, the question is whether it is possible, on the basis of box-averaged cross sections, to calculate the average quantities, primarily the box average power distribution.

The production of box-averaged, few-group cross sections at Risø at present generally takes place on the basis of box calculations with the CDB[3] code. A single box is taken out, compare fig. 3.a, with or without control rod, and calculated with reflecting boundary conditions. The average cross sections are determined on the basis of flux volume weighting of the cross sections of the different regions of the box. The generation of the different group cross sections is quite straight-forward by the flux volume weighting method, used to save the reaction rates and thus the reactivity of the box. The average diffusion constants are at present homogenized inversely, i.e. the transport cross sections are flux volume weighted as the other group

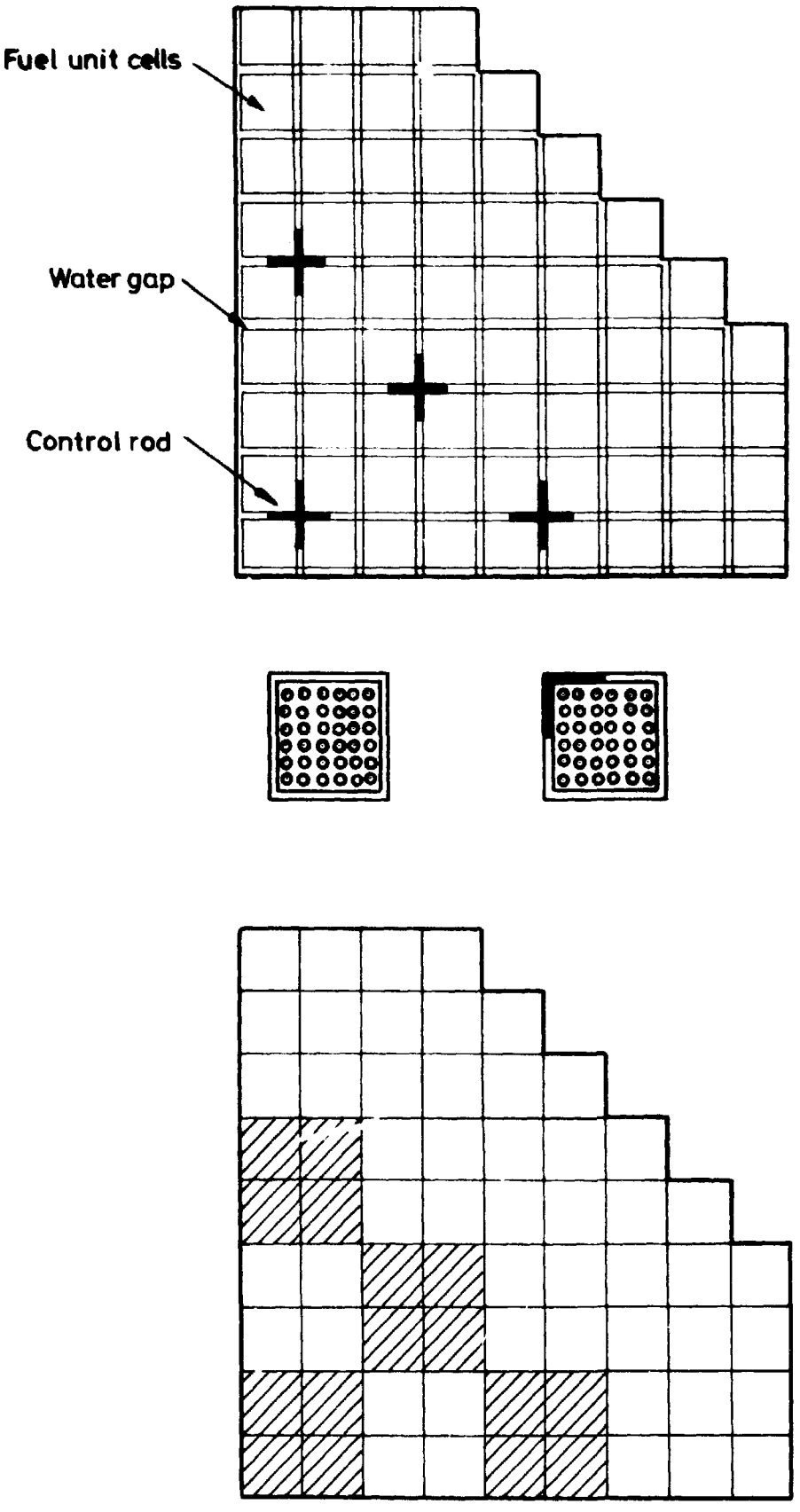


Fig. 3.a. Box homogenization for the overall calculation, on a quarter of a reactor core.

cross sections. Another possibility will be described later in this chapter.

An unfavourable aspect of this method for production of box average cross sections is that the flux spectrum in the box is calculated for a separate box, i.e. the surrounding boxes do not affect the spectrum, especially for the rodded fuel box this is a severe restriction as in most cases only a few of the boxes in a reactor are rodded.

A last problem is how severely the smearing out of the fuel boxes, especially that of the control rod over a large region, in practice 4 fuel boxes representing several diffusion lengths, affects the overall power distribution.

First let us look at the problem of determining the proper diffusion constants. As mentioned earlier the average diffusion constants in the standard CDB version are found from the flux volume weighted transport cross section, i.e.:

$$\bar{D}^g = \frac{1}{3\,\bar{\Sigma}^g_{tr}} , \tag{3.1}$$

where g is the group index. However, it has been observed that the influence of strong absorbers, as for example control rods, is over-estimated in this homogenization method. For that reason an alternative homogenization method was investigated. The method is based on the following two principles: (1) conservation of the reaction rates, which is obtained by using the same group cross section homogenization as in the CDB method; and (2) conservation of the average free mean path, which is obtained by flux volume weighting of L^2, when the average value of L^2 is found, the diffusion constant is determined by multiplying $\bar{L}^2$ by the average absorption cross section $\bar{\Sigma}_a$:

$$D^g = \bar{L}^{g^2} \cdot \bar{\Sigma}^g_a \tag{3.2}$$

The L^2 method is simply presented as a proposal, and no further theoretical argumentation will be given. However, it may be mentioned that when the regions in the box are nearly homogeneous, the two methods will give identical diffusion constants, as in this case $\bar{L}^{g^2} \sim \bar{D}^g/\bar{\Sigma}_a$. For realistic fuel boxes the diffusion constants obtained by (3.2) are normally somewhat larger than those obtained by (3.1), increasing the coupling between the boxes in the overall calculation. It can be reported that for all test calculations performed both with homogenization of fuel boxes for the Dresden 1 reactor and with many academic examples, the power distributions obtained by the L^2 method were always somewhat better than those of the ordinary methods compared with the results obtained by direct represention of all regions in

the overall calculation. Especially the power sharing between rodded and unrodded fuel boxes is improved.

In addition to the problem of determining the proper average cross sections and diffusion constants the question is whether it is possible to calculate the overall power distribution on the basis of the smeared out cross sections. In the limite where the whole reactor is homogenized and represented by one set of cross sections it is naturally impossible to calculate the overall power distribution. Whether four fuel boxes surrounding a control rod is a too large unit for homogenization has been investigated by calculations on several reactor configurations. In fig. 3. a a typical quarter core configuration is shown with control rods inserted in the central part of the core. In the case with smeared cross sections the discrete control rods are replaced by large grey regions. Several calculations on different reactor configurations with control rods in the central part of the core seem to show that the calculated power level is 10-20% lower in the central part of the reactor when smeared cross sections are used than in the case of direct representation. The use of diffusion constants determined by the L^2 method does improve the results, but not enough. There seems to be two ways to tackle the problem. Either simply to avoid to smear out the control rods over regions as large as four fuel boxes or to use some sort of fitted control absorption cross section, i.e. for example multiply the thermal control absorption cross section by a smearing out constant less than unity.

4. Comparison between Calculated and Measured Box-averaged Power Distribution for the Dresden 1 Reactor, Initial Half Power Conditions

The investigations described in the preceding chapters were all set up in order to fulfil the requirements of proper cross sections for the 3-dimensional overall calculations. In ref. 1 a series of calculations performed on the Dresden 1 reactor with the Risø reactor code complex is described. The calculations consist of pin cell and box burn-up calculations and full 3-dimensional overall calculations inclusive of hydraulics; the calculations were compared with the few measurements available. The initial half power box average power distribution has been measured and reported. However, the calculated power distribution does not agree satisfactorily with the measurements. In the old calculations of ref. 1 the overall code SYNTRON[2)] could only treat one quarter of the core and rather limited number of hydraulic channels. As no quarter core symmetry exists in the control rod pattern, this was a severe restriction. For that reason the SYNTRON code has been

modified so that it is now possible to handle as much as about 50 x 50 x 50 mesh points, naturally dependent on the number of trial functions used in the synthesis solution. For static calculations without hydraulics as much as 70 x 70 x 70 mesh points are possible. Furthermore the possible number of hydraulic channels has been increased to 50-100. It is thus possible now to set up whole-core calculations with the SYNTRON/VOID code.

In this chapter a description is given of the methods used in setting up a whole-core calculation with the SYNTRON/VOID code on the Dresden 1 half power initial example.

The basic neutron data are as in the calculations of ref. 1 taken from the SIGMA MASTER TAPE. However, the data processing code CRS[4, 5] has been modified and improved since the calculations of ref. 1. These modifications are fully described in ref. 5, and they will naturally affect the results to some degree. The modifications used in CRS for these calculations are: A correction to the removal cross sections of H in the resonance region has been implemented. This correction was only used for water near fuel pins, i.e. pin cell water and the water surrounding the fuel box, but not for reflector water. The thermal scattering matrices are generated by the new NELLY routine. NELLY calculates the scattering matrices on the basis of an interpolation in the NELLY library in 35 energy groups; this library has originally been calculated by the NELKINSCM routine in 205 energy groups and afterwards condensed to the present NELLY library. The spectrum calculation is CRS in 76 energy groups for the condensation of the microscopic pin cell cross sections to 10 groups to be used in CDB was set up as a three-region collision probability calculation with the GEPUR routine, i.e. the homogeneous pin cell spectrum calculation in 76 groups in CRS used in ref. 1 was replaced by the more elaborate heterogeneous spectrum calculation. The last two changes, NELLY and the 3-region spectrum calculations, seem only to affect the box calculations slightly, whereas the H removal correction lowers the k_{eff}'s by about 0.5%.

The one-dimensional collision probability calculations for the inter-box water and control rod cross sections were set up quite similarly to the description in ref. 1, only now within the CRS program, and the H removal correction and NELLY routine are applied.

These are the methods used for the cross section supply of the CDB box code for the calculations described in this report. The fuel box calculations are otherwise performed as described in ref. 1, 10 energy groups for the pin cell and 5 groups for the box overall. In connection with the calculation of a γ-matrix with the HECS[6] code two things ought to be mentioned. The HECS calculation is performed on the same geometry as used in CRS for the

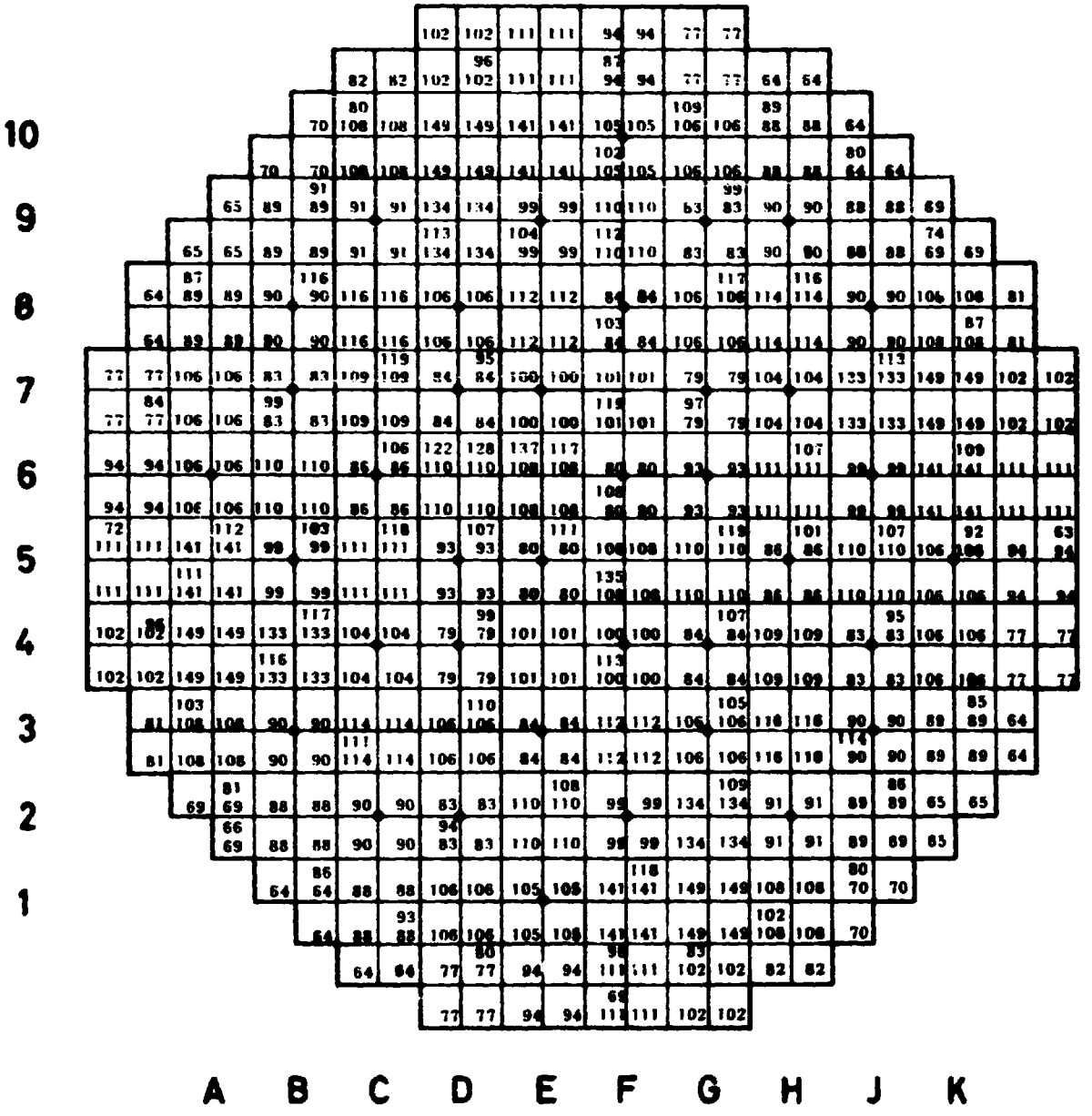
calculation of the corresponding effective cross sections. The transport cross sections used by HECS are condensed by CRS from the 76 groups to the perhaps 5 groups of HECS by simple flux weighting. This is in contrast to the condensation used when the transport cross sections are to be used for diffusion constants. In that case the condensation is performed by inverse flux weighting of the transport cross section. If this difference is not taken into account, it might cause severe errors in the succeeding box calculation.

It should be mentioned that the box average cross section used for the following 3D overall calculation was calculated on the basis of box calculation where all regions are cross-section-represented. This is due to the fact that the homogenization routine in the present version of CDB cannot produce correct average cross sections for a fuel box containing γ-matrices.

On the basis of these improvements a full core calculation was set up with the SYNTRON/VOID program on the initial half power situation for the Dresden 1 reactor. The example is described in ref. 10, and measurements of the total fuel assembly power distribution are reported. The gamma probe measurements were performed after an initial short run at a steady power of about one half of the rated power. The total mass flow was likewise of about half the rated value. The measurements were made with essentially zero exposure of the fuel. The control rod pattern is given in ref. 10. The full description of the reactor core, dimension, material compositions, and so on is given in ref. 1. The control rods in Dresden 1 have 13 possible notch positions, 0 fully inserted and 12 fully withdrawn. The degrees of insertion of the different control rods are listed in fig. 4.b. The control rods inserted are shown as dots in figs. 4.a and c.

The following 3-dimensional SYNTRON/VOID calculation was set up on the example. Only 2 energy groups were used. The number of mesh points used was 48 x 48 in the radial directions and 36 in the axial direction. The mesh points are all placed inside the core as the reflector is represented by a gamma matrix. Static 2-dimensional test calculations with a varying number of mesh points have shown that the error introduced by using only 48 x 48 mesh points is small as long as the reflector is represented by gamma matrices. Only two trial functions in each energy group were used. The Doppler effect was accounted for in the same fashion as described in ref. 1. The hydraulic data used are similar to the data used in ref. 1. However, the number of hydraulic channels used are now as many as 60, which in fact for the present case is one channel for every four fuel boxes, taking into account a half core rotational symmetry of the core.

Top: measurement
Bottom: calculation



Average box power 100

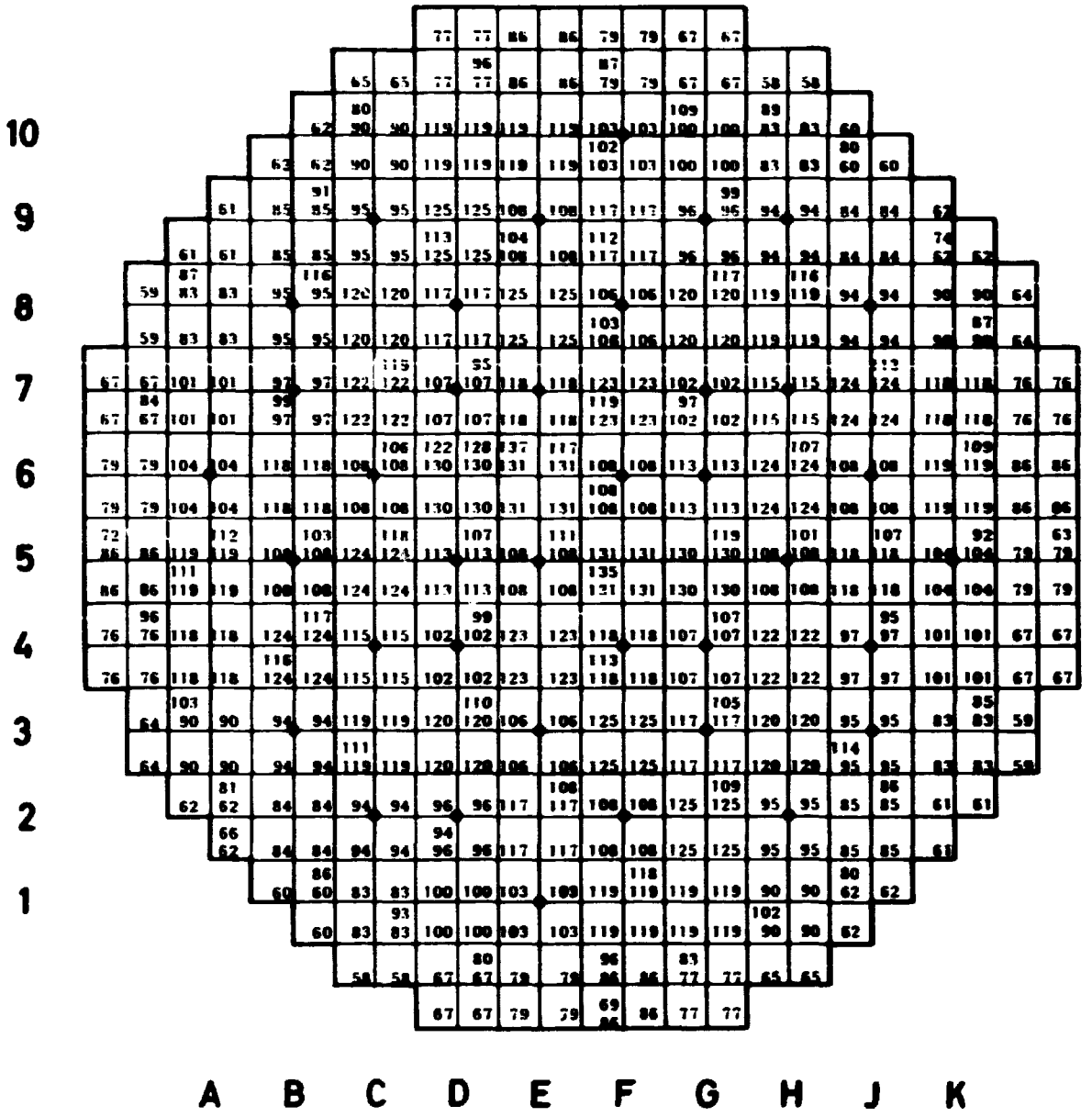
Fig. 4.a. Dresden 1, initial half power box average power distribution

10						4				
9			0		0		0	9		
8		9		2		0			0	
7		0		0	5		0	2		
6	4		0			0	5		0	
5		0		5	0			0		4
4			2	0		5	0		0	
3		0			0		2		9	
2			9	0		0		0		
1				4						
	A	B	C	D	E	F	G	H	J	K

Fig. 4.b. Control rod notch positions for the Dresden 1 initial half power case

In fig. 4.a the calculated box average power distribution compared with the measurements is shown. The box average power is found by axial integration of the 3D power for each fuel box. The diffusion constants used are generated by the L^2 method. It will be seen that the power sharing between rodded and unrodded boxes is quite satisfactory compared with the measurements. However, as predicted in the preceding chapter, the average power in the middle of the core is calculated too low because of the smeared control rods. Because of this over-estimating of the absorption in the smeared control rods the calculation was repeated with modified thermal absorption cross sections for the smeared control rods; a $\Delta \Sigma_a^2$ of 0.007 cm^{-1} was simply subtracted from all the control rod thermal absorption cross sections. The obtained power distribution is shown in fig. 4.c. For this case the agreement between the calculation and the measurements is much better.

Top: measurement
Bottom: calculation



Average box power 100

Fig. 4.c. Dresden 1, initial half power box average power distribution. Modified control rod absorption cross section.

5. Conclusion

The following conclusions may be drawn from these investigations. The smearing-out of control rods over the adjacent four fuel boxes is prohibitive. The use of the L^2 method for the determination of the diffusion constants does improve the power sharing between rodded and unrodded fuel boxes. However, 3-dimensional calculations based on box average cross sections determined on the basis of separate box calculations, are not expected to give satisfactory results unless some experimentally determined modifications are put on the smeared control absorption cross section. The use of gamma-matrix representation of the reflector is strongly recommended.

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